

A CONCEPTUAL AND NUMERICAL MODEL FOR REACTION-TRANSPORT PROCESSES IN UNSATURATED FRACTURED ROCK AT YUCCA MOUNTAIN: MODEL VALIDATION USING THE DRIFT SCALE HEATER TEST. E. L. Sonnenthal¹, N. F. Spycher², J. A. Apps³, and M. E. Conrad⁴, ¹Earth Sciences Division, E. O. Lawrence Berkeley National Laboratory, MS90-1116, elsonnenthal@lbl.gov, ²nspycher@lbl.gov, ³jaapps@lbl.gov, ⁴MS70A-4418, msconrad@lbl.gov.

Introduction: We have developed a conceptual and numerical model to predict the evolution of the geochemical system around the potential nuclear waste repository in the unsaturated zone at Yucca Mountain, NV [1]. The Drift Scale Test (DST), initiated in Dec. 1997, is the primary large-scale thermal test used for the validation of numerical models of coupled thermal, hydrological and chemical (THC) processes at Yucca Mountain. The test has resulted in maximum rock temperatures of about 200°C and has been closely monitored *in situ* through the collection of gas and water samples as well as thermal and mechanical measurements. Here we present a description of the model and describe the results of simulations and comparisons to measured gas and water chemistry.

Conceptual and Numerical Models: The evolution of the chemical regime in the unsaturated zone surrounding a heat source is closely related to the spatial distribution of temperature and the transport of liquid water and vapor. An important aspect of the unsaturated fractured tuff at Yucca Mountain is that the highly permeable fractures are nearly dry, and the low permeability rock matrix (porosity ~10%) has a water saturation of about 90%. Thus, heating of the rock induces boiling of the matrix pore water, vapor transport into fractures, and condensation on fracture walls. A dryout zone extends outward from the heat source, surrounded by a boiling zone, then by a condensation zone. A fracture drainage zone extends for at least tens of meters beneath the heat source.

A numerical model for reaction-transport processes in the fractured welded tuffs must account for the different rates of transport in fractures, compared to a much less permeable rock matrix. Transport rates greater than the rate of equilibration via diffusion leads to disequilibrium between waters in fractures and matrix. In an unsaturated boiling system the transport of gaseous species, especially CO₂, is important. Compared to typical reaction-transport models where the system is wet everywhere, special treatment must be made for the transition to areas that are completely dry. The model must also capture the differences in mineralogy in fractures and matrix, and their evolution. To handle these separate yet interacting processes in fractures and matrix, the dual permeability method has been extended, such that each gridblock is broken into a matrix and fracture continuum, characterized by its own pressure, temperature, liquid saturation, water and gas chemistry, and mineralogy. Our simulations of THC processes include coupling between heat, water, and vapor flow, aqueous and gaseous species transport, kinetic and equilibrium mineral-water reactions, and

effects of mineral precipitation/dissolution on porosity, permeability, and capillary pressure in two dimensions. Aqueous species included are H⁺, Ca²⁺, Na⁺, K⁺, SiO₂(aq), Mg²⁺, Al³⁺, Fe³⁺, SO₄²⁻, HCO₃⁻, Cl⁻, and F⁻. Minerals include silica phases (α-cristobalite, quartz, tridymite, amorphous silica, and opal-CT), calcite, feldspars, smectites, illite, kaolinite, zeolites, fluorite, iron oxides, and gypsum. Treatment of CO₂ includes gas-water equilibration, diffusion and advection.

Evolution of Gas and Water Chemistry: The thermohydrological regime results in zones of differing chemical environments characterized by dilution or by concentration caused by boiling. Comparisons between observed and modeled gas phase CO₂ concentrations show that the model captures overall trends in gas phase transport and reactions as well as the effects of CO₂ on pH of draining high temperature waters. Comparison with measured aqueous species concentrations show that there is little interaction of fracture water with matrix pore water but that reactions with fracture-lining minerals such as calcite, silica polymorphs and k-feldspar are significant. Isotopic studies have shown the effects of calcite dissolution in drainage zones, which is supported by the model results (Figure 1).

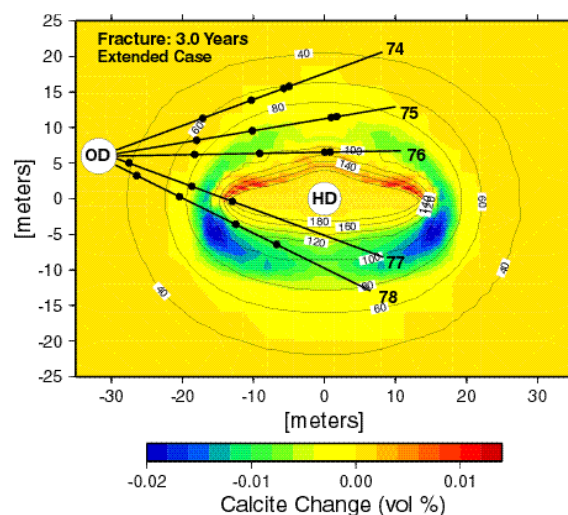


Figure 1. Modeled change in fracture calcite and temperature for a cross section through the DST. Monitoring boreholes overlain. (HD = heater drift, OD = observation drift).

References:

- [1] Sonnenthal E. and Spycher N. (2000) *Lawrence Berkeley National Laboratory, Report LBID 2340.*